Implementation of CG Method on GPU Cluster with Proprietary Interconnect TCA for GPU Direct Communication

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Outline

- Background and Motivation
- TCA (Tightly Coupled Accelerators) Architecture
- Collective Communication
  - Allgather and Allreduce
- CG Method
- Conclusion

Background

- GPU clusters are common as HPC systems
  - High peak performance / cost ratio
  - High peak performance / power ratio
- **Strong scaling** on GPU clusters is difficult.
  - Large gap between computation perf. and communication perf.
  - Communication latency between GPUs is larger than between CPUs
- Improving communication performance between GPUs is demanded for HPC
  - Our target is to develop a direct communication system between GPUs over different nodes for future accelerated computing
    ⇒ Tightly Coupled Accelerators (TCA) architecture

Our Previous Work on TCA

1. "**Tightly Coupled Accelerators Architecture for Minimizing Communication Latency among Accelerators**," In *AsHES 2013*.
   - Introduction (descriptions) on the TCA architecture
   - Performance evaluation on the ping-pong communication of TCA
2. "**QCD Library for GPU Cluster with Proprietary Interconnect for GPU Direct Communication**," In *HeteroPar 2014*.
   - Application of TCA to improve the communication performance in QUDA QCD library

Motivation

- Further performance evaluation of TCA
- Implementing **CG method** by using TCA
  - CG method: Iterative solution for systems of linear equations
  - Implementing **allgather and allreduce collective communication** with TCA API
- Evaluating the performance and seeing how TCA is effective

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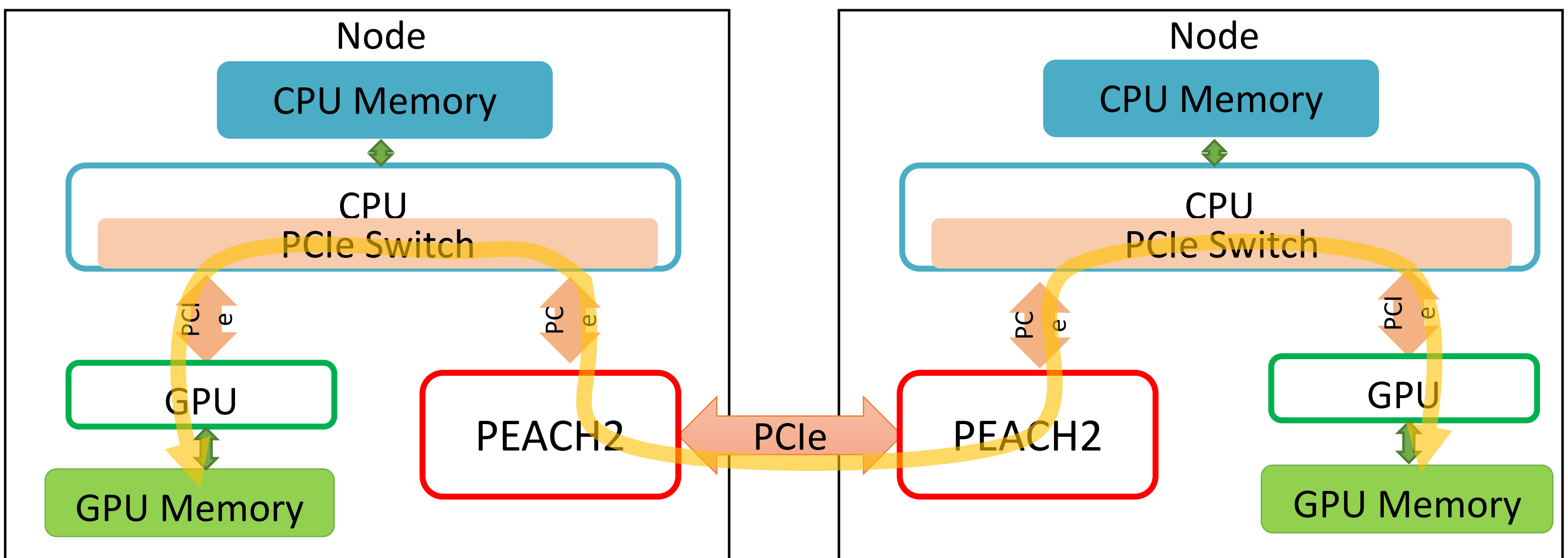
TCA (Tightly Coupled Accelerators) Architecture

- Technology for direct connection between accelerators (GPUs) over different nodes without CPU assistance.
  - Low communication latency
    - By eliminating extra data copy to the host (CPU)
    - Improves strong scalability



PEACH2

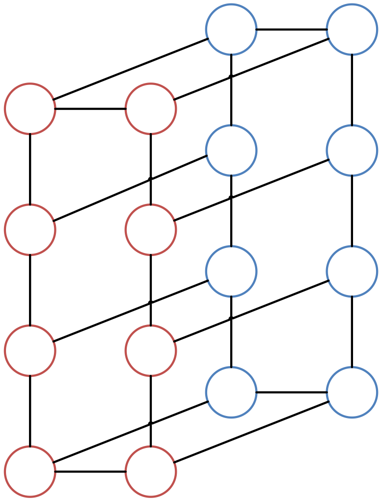
- PCI Express Adaptive Communication Hub ver. 2
- Implementation of TCA by FPGA
- Enables direct connection between GPUs with **PCI-Express (PCIe)** technology
  - Direct data copy is accomplished by NVIDIA GPUDirect Support for RDMA (GDR)
  - Protocol conversion is not required

    ⇒ Lower latency than InfiniBand
- Contains 4 PCIe ports (3 external ports)
  - Each port has **PCIe Gen2 x8** bandwidth (4 GB/s peak)
- NOTE: For convenience, we call this implementation of TCA on PEACH2 as "*TCA*".

HA-PACS/TCA

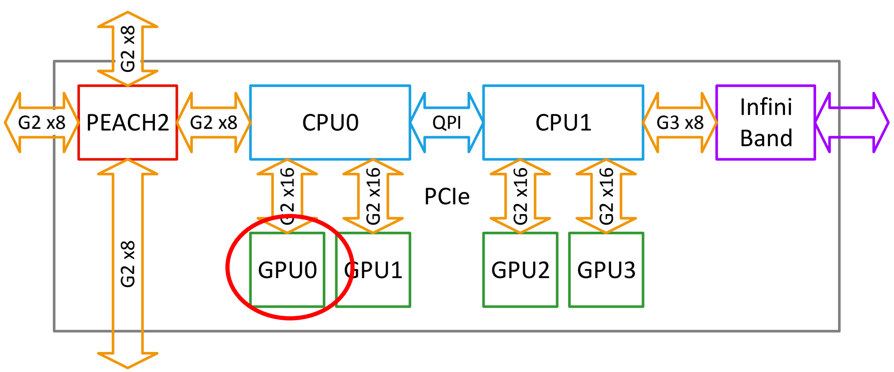
- Proof-of-concept GPU cluster of TCA concept in HA-PACS project

- 64 compute nodes in total
  - 4 sub-clusters each of which consists of 16 nodes
  - PEACH2 is equipped with
    - Sub-cluster configures 2x8 ring (torus) network.
      - By connecting 3 neighbor nodes through 3 PCIe ports of PEACH2
  - MPI communication through InfiniBand is also possible.
    - Can be considered to be a normal GPU cluster
    - Full-bisection bandwidth fat-tree network.



Performance Evaluation Condition

- Evaluation on a sub-cluster of HA-PACS/TCA
  - Up to 16 nodes (processes)
  - Using 1 GPU / node



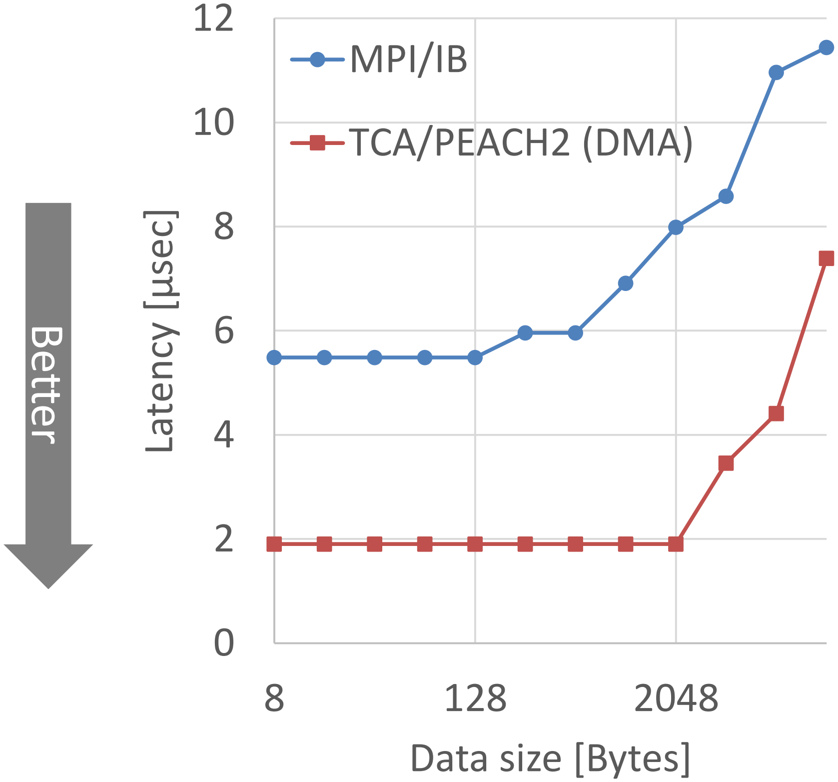
Hardware	
CPU	Intel Xeon E5-2680 2.8 GHz × 2 (**IvyBridge** 10 cores / CPU)
GPU	NVIDIA Tesla K20X × 4 (**Kepler GK110** 2688 cores / GPU)
TCA	**PEACH2 board** (Altera Stratix-IV GX 530 FPGA)
InfiniBand	Mellanox Connect-X3 Dual-port QDR
Software	
CUDA	6.5
MPI	MVAPICH 2 GDR 2.1a
C Compiler	Intel Compiler 14.0.3

MPI (MVAPICH2-GDR)

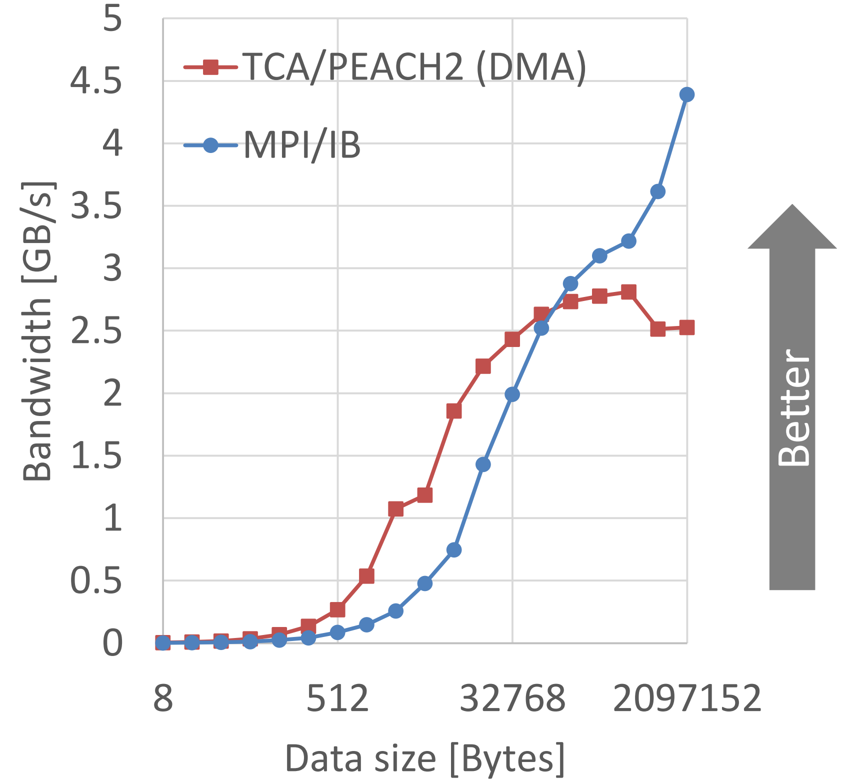
- We compare the performance of implementation using TCA with using MPI communication.
- MPI Impl.: **MVAPICH2-GDR 2.1a（MV2GDR)**
  - MPI implementation for InfiniBand
  - As with TCA, MV2GDR utilizes GPU Direct for RMA (GDR) to improve latency and bandwidth for small data communication

Ping-pong GPU-to-GPU Communication Performance

Latency



Bandwidth



- TCA/PEACH2 is better for small sizes.
- For large sizes, TCA is outperformed by MPI/IB since the difference of peak bandwidth perf. (4 GB/s vs. 8 GB/s) → **How about collective communications?**

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TCA Implementation of Collective Communication

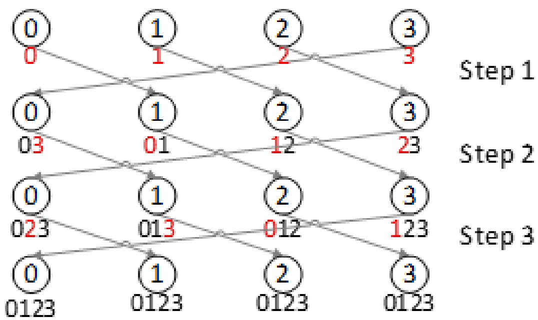
- **Allgather**
  - All processes gather data of each process.
  - Gathering data of KB-MB order
    - Communication bandwidth as well as latency is important.
- **Allreduce**
  - Conducts specified operation (sum, max, …) among data arrays (x_i) of each process and store the reduction result in all processes.
  - Targeted for CG method, we implement and tune allreduce (sum) for double-precision scalar (8 Bytes) data.
    - $(x_0 + x_1 + x_2 + x_3 = \sum_{i=0}^{3} x_i)$
    - Latency decides the performance.

Algorithms for Collective Communication

- Implement and evaluate 4 algorithms

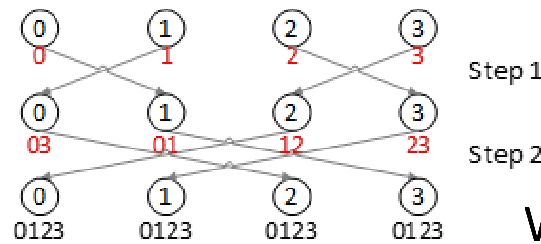
1. Ring algo.

Communication steps: p-1



3. Recursive Doubling algo.

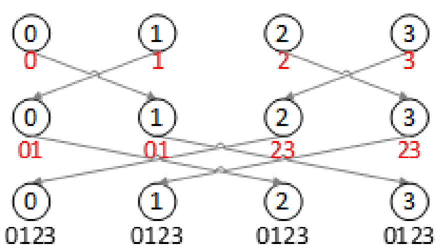
Communication steps: $\log_2 p$



We suppose #processes (p) is in power of 2.

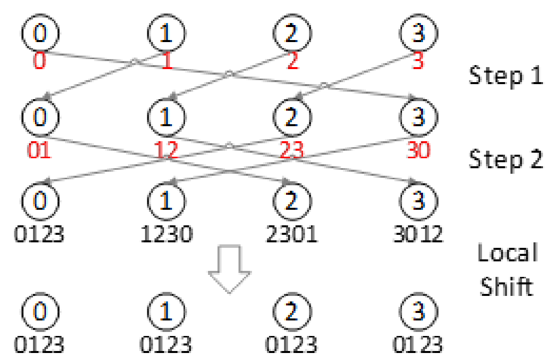
2. Neighbor Exchange algo.

Communication steps: p/2



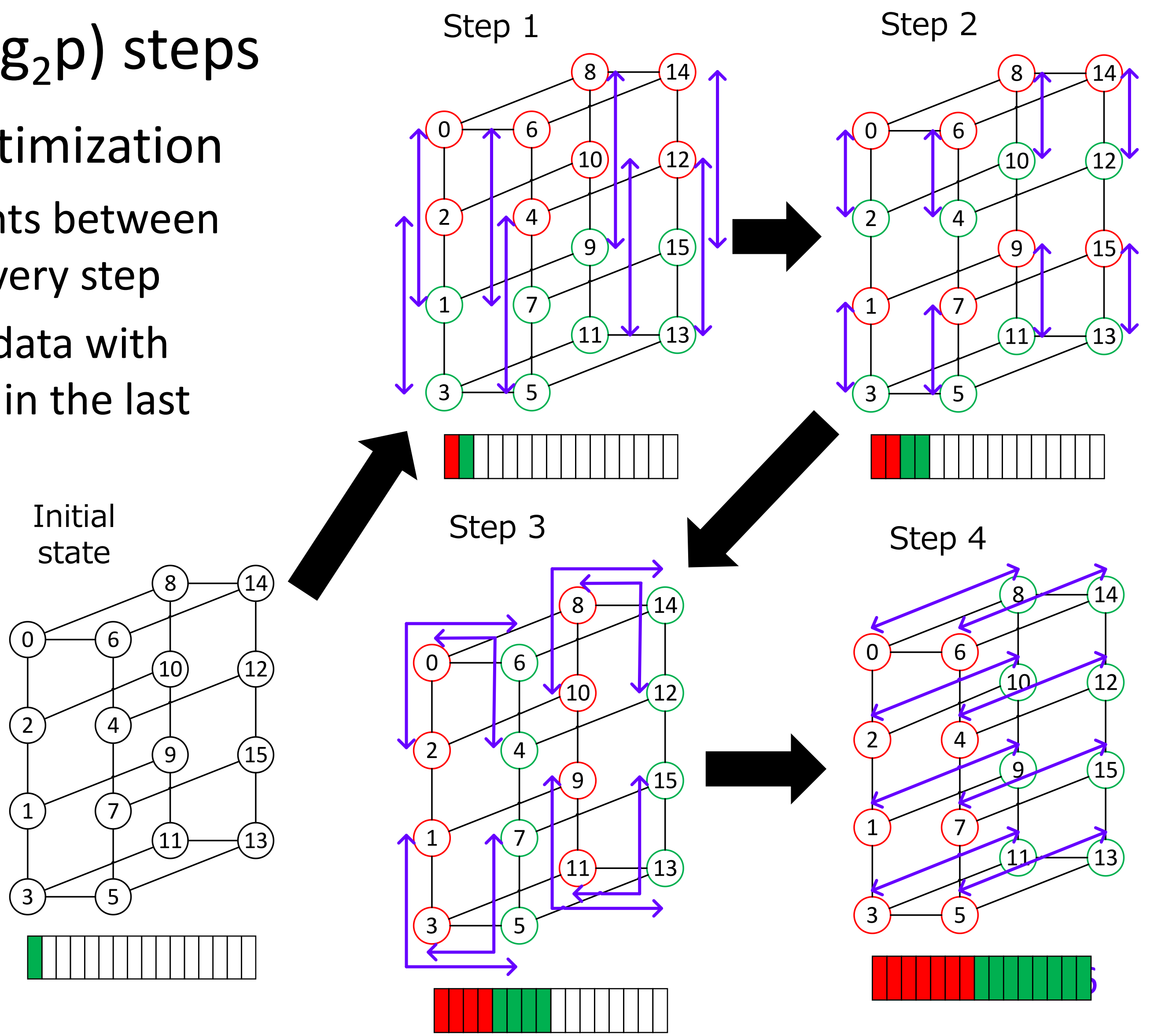
4. Dissemination algo.

Communication steps: $\log_2 p$

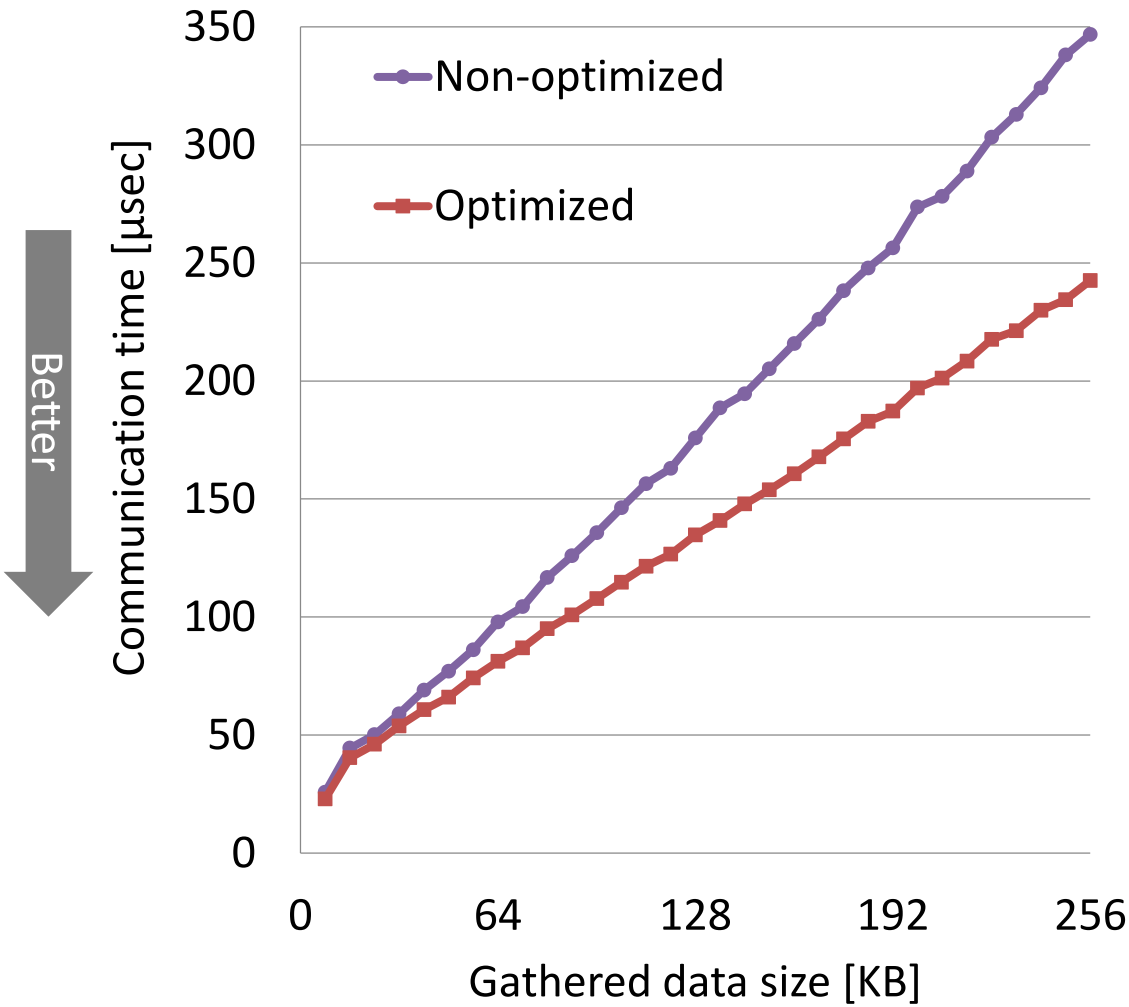


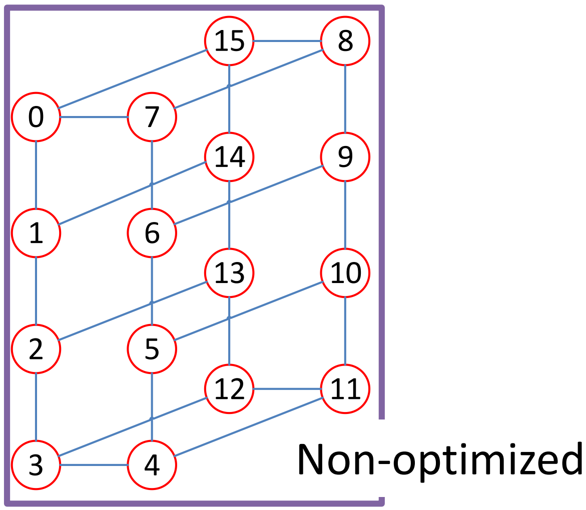
Allgather Implementation: Recursive Doubling (In case #processes = 16)

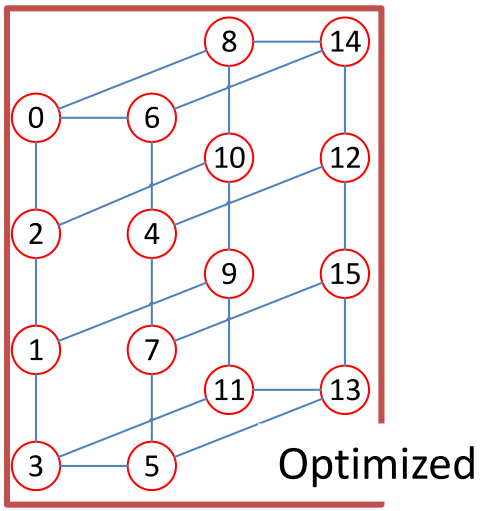
- Requires 4 (= $\log_2 p$) steps
- Node mapping optimization
  1. Same hop counts between any nodes in every step
  2. Communicate data with neighbor node in the last step



Impact of Node Mapping to Allgather Performance (#Processes=16)

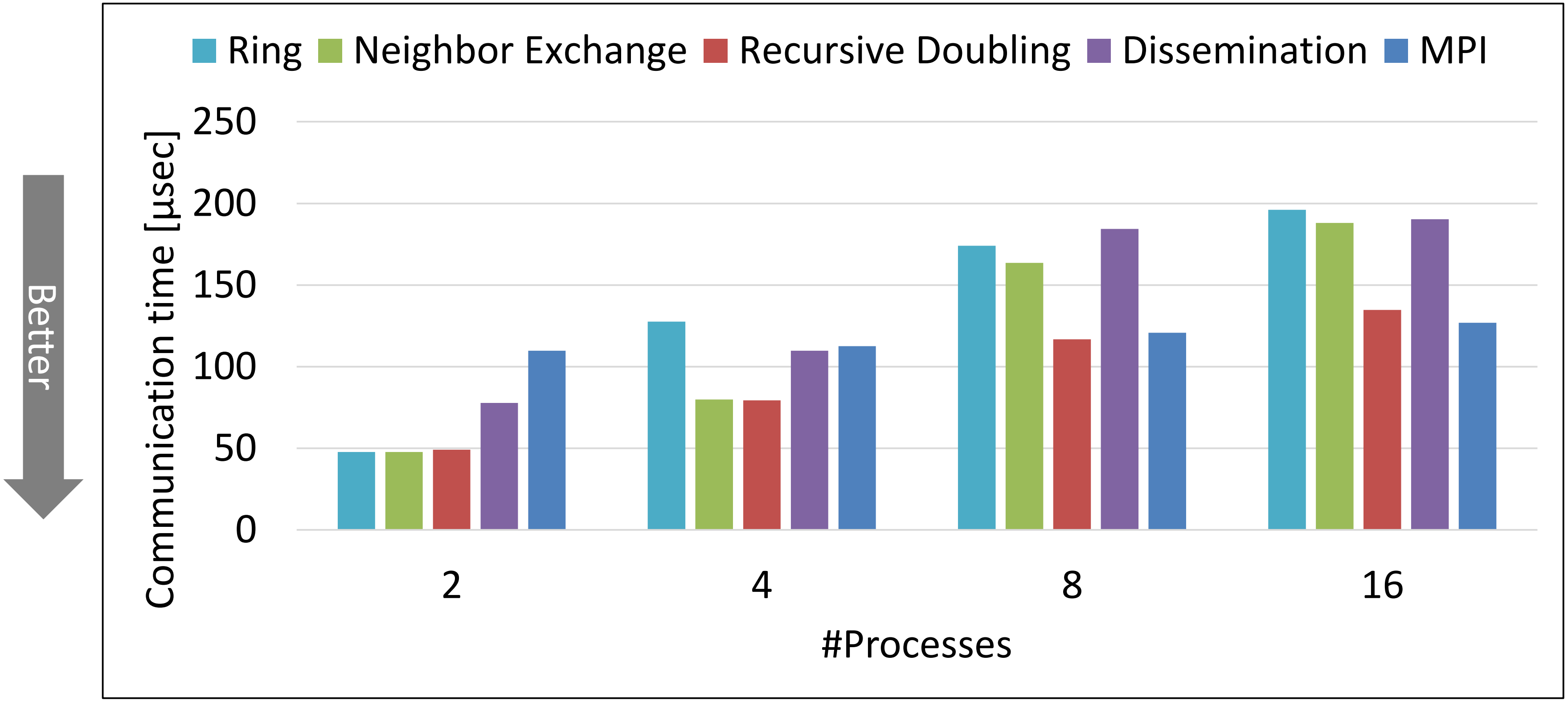




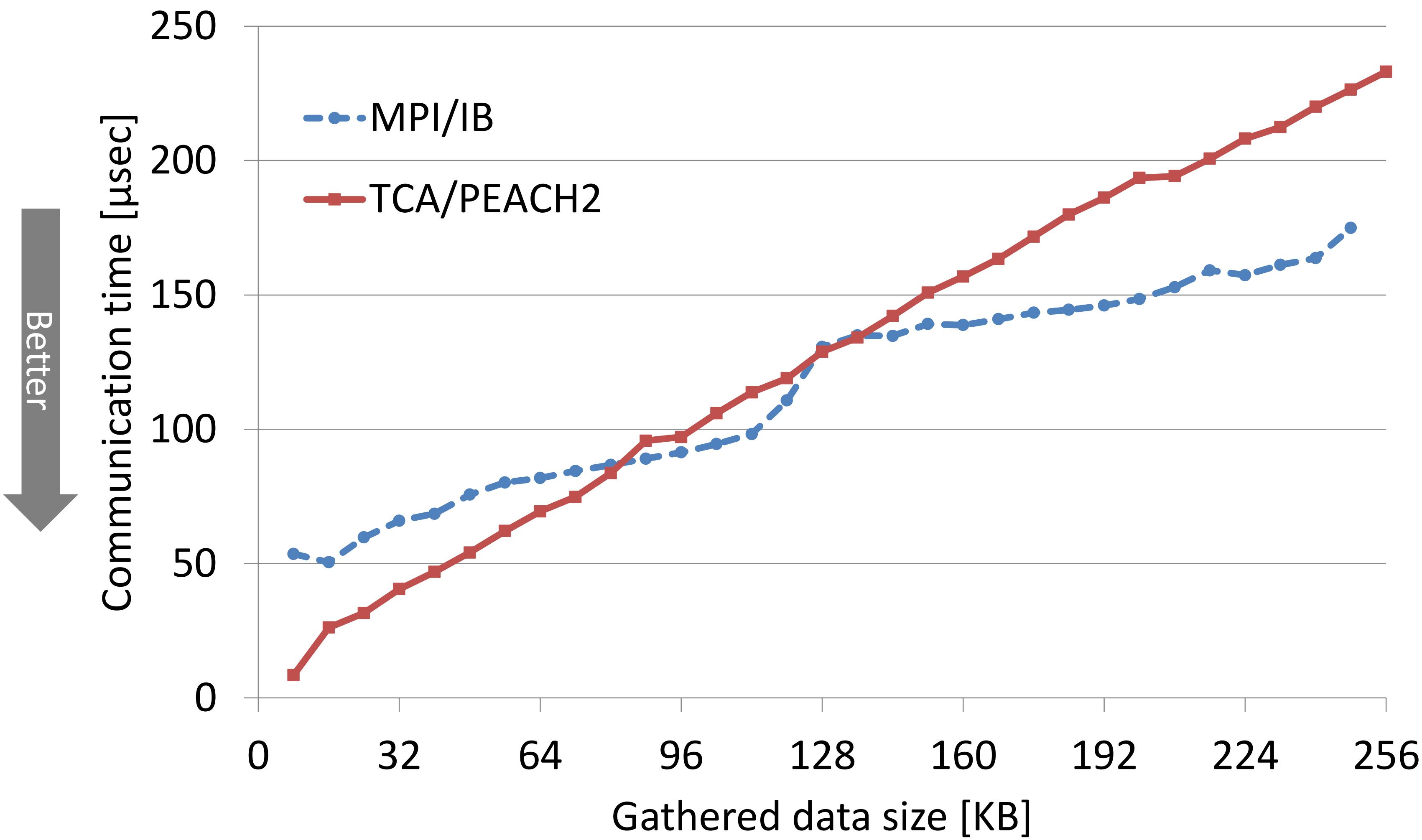


Allgather Perfomance Comparison among Different Algorithms

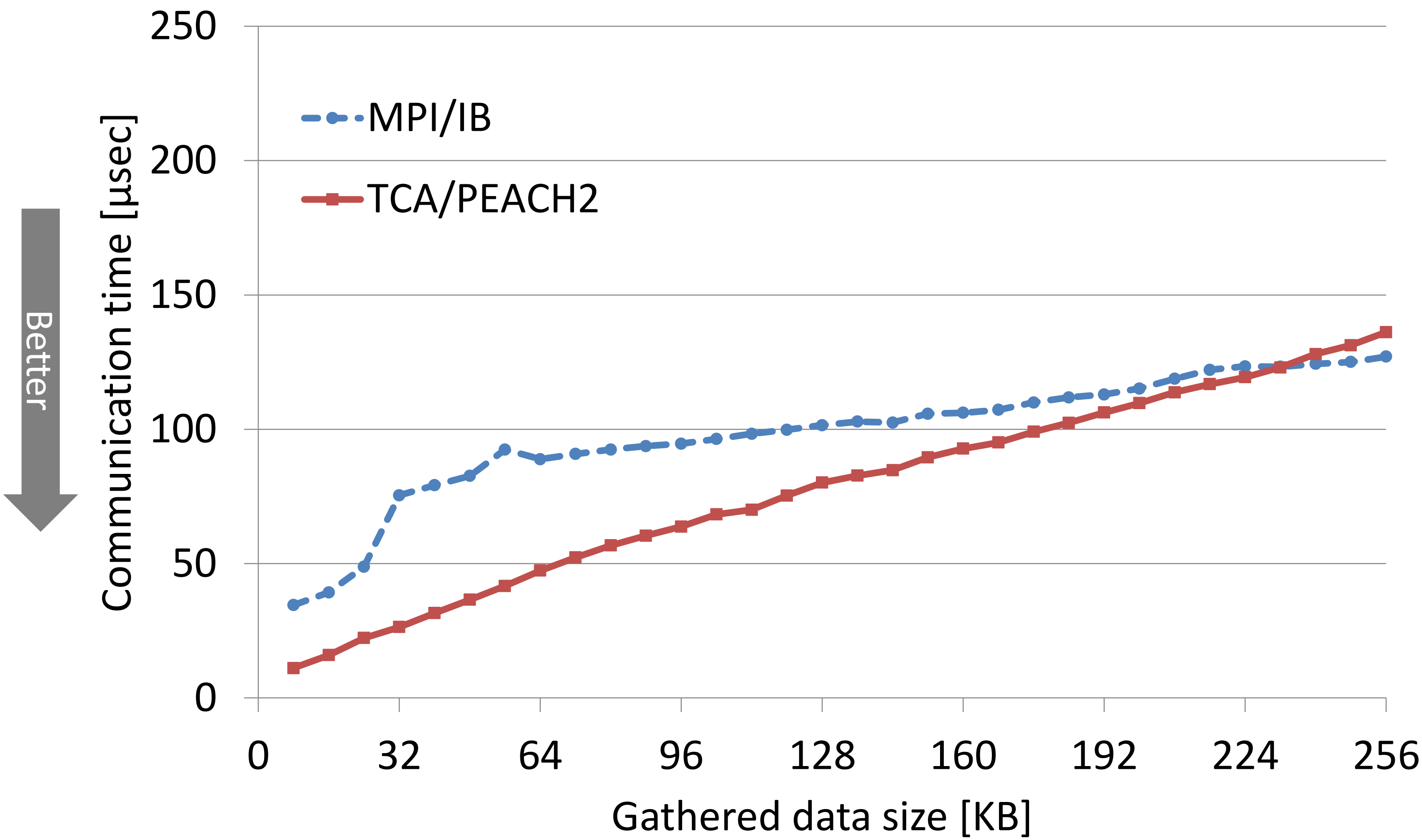
- Time for all-gathering **128 KB** data
  - N=16384 case in CG method
- **Recursive Doubling shows good performance**
  - However, when p=16, TCA is slower than MPI for this size



Allgather Performance (#Processes=16)

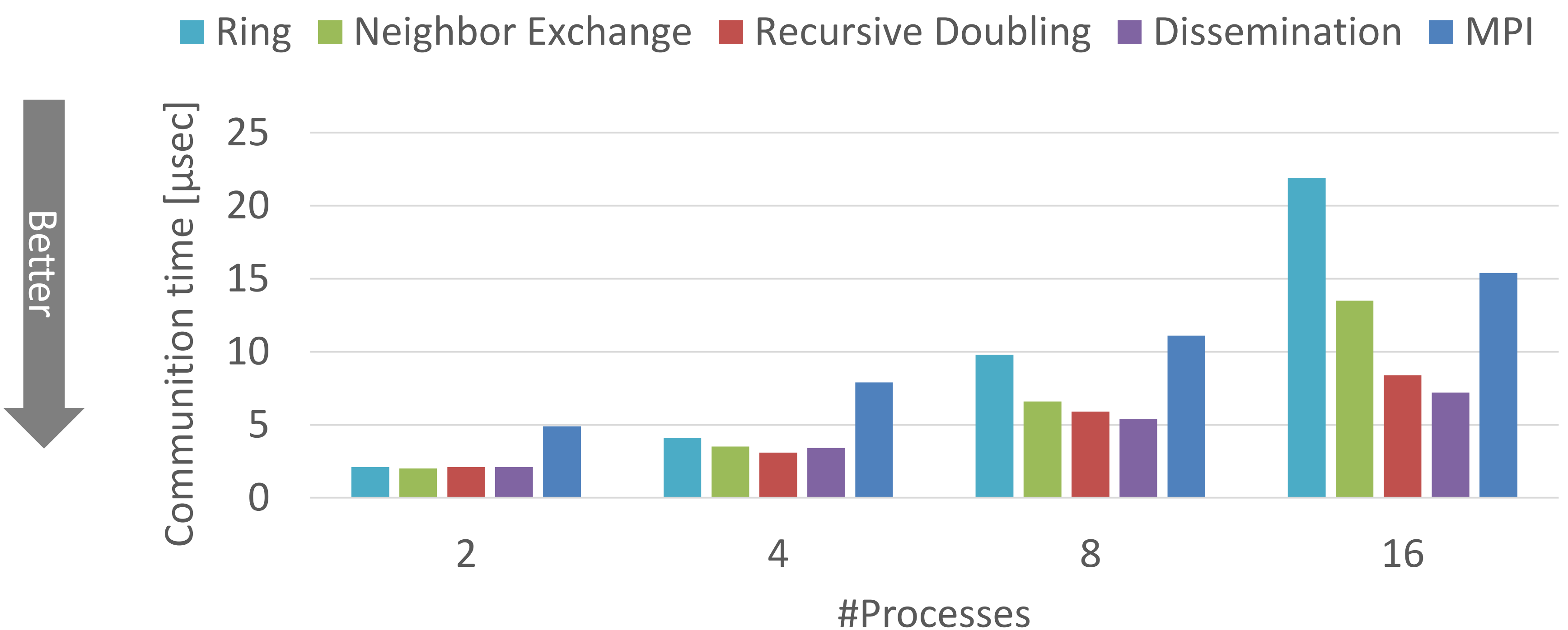


Allgather Performance (#Processes=4)



Allreduce Performance

- CPU-to-CPU allreduce time for 8 Bytes scalar data
- **Dissemination algorithm is the fastest.**
- TCA/PEACH2 is **more than 2x faster** than MPI/IB
  - Low latency of TCA works effectively



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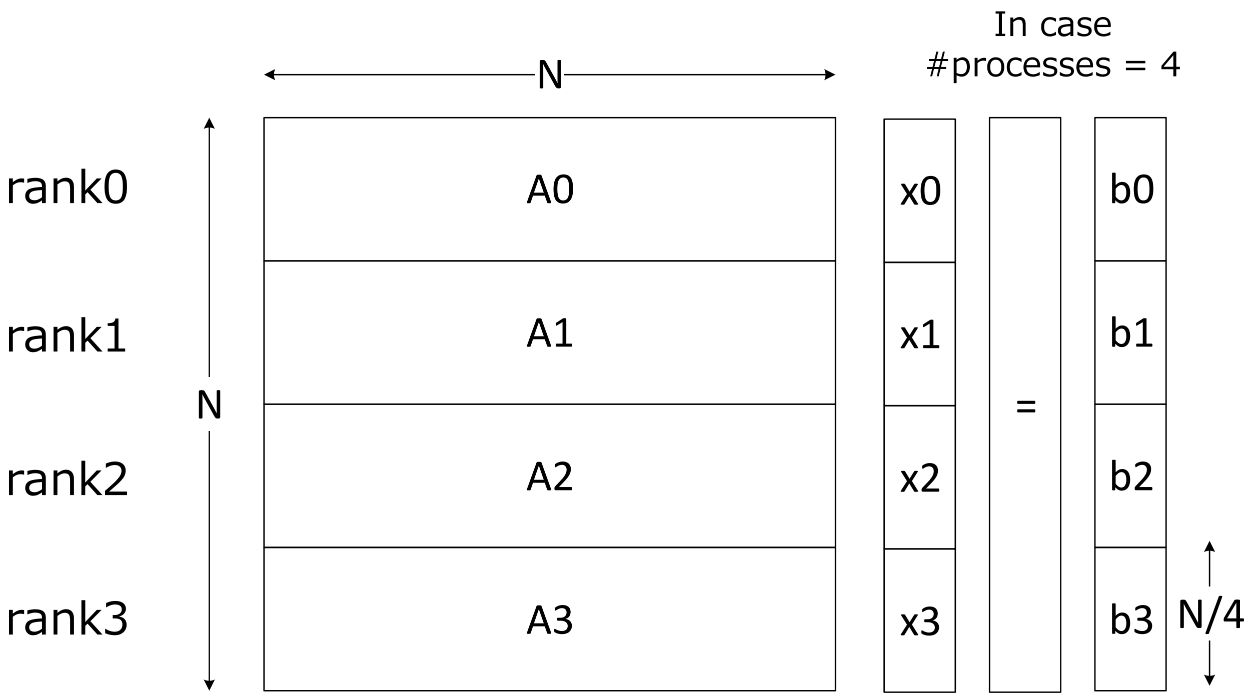
CG (Conjugate Gradient) Method

- Iterative solution for systems of linear equations
  - $Ax = b$
    - A: N-by-N symmetric positive-definite matrix (sparse matrix)
      - Sparse matrix is stored in **CRS (Compressed Row Storage)** order.
    - x, b: N-dimensional vector
  - No preprocessing
- Main computation parts (NVIDIA's **cuSPARSE** and **cuBLAS** are utilized)
  - **SpMV** x1 – Sparse Matrix-Vector Multiply ($\boldsymbol{q} := A\boldsymbol{p}$)
  - **DOT** x3 – Vector Dot Product ($\alpha := \boldsymbol{p}^T\boldsymbol{q}$)
  - **AXPY** x3 – Vector Multiply-Add ($\boldsymbol{y} := \alpha\boldsymbol{x} + \boldsymbol{y}$)

$$
\begin{array}{l}
\boldsymbol{r} := \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x} \\
norm0 := \mathrm{sqrt}(\boldsymbol{r}^T\boldsymbol{r}) \\
\textbf{for } k := 1, 2, \cdots \textbf{ do} \\
\quad \rho := \boxed{\boldsymbol{r}^T\boldsymbol{r}} \\
\quad \textbf{if } k = 1 \textbf{ then} \\
\quad\quad \boldsymbol{p} := \boldsymbol{r} \\
\quad \textbf{else} \\
\quad\quad \beta := \rho/\rho\mathrm{prev} \\
\quad\quad \boldsymbol{p} := \beta\boxed{\boldsymbol{p} + \boldsymbol{r}} \\
\quad \textbf{end if} \\
\quad \boldsymbol{q} := \boxed{\boldsymbol{A}\boldsymbol{p}} \\
\quad \alpha := \rho/\boxed{(\boldsymbol{p}^T\boldsymbol{q})} \\
\quad \boldsymbol{x} := \boxed{\alpha\boldsymbol{p} + \boldsymbol{x}} \\
\quad \boldsymbol{r} := \boxed{-\alpha\boldsymbol{q} + \boldsymbol{r}} \\
\quad norm := \mathrm{sqrt}\boxed{(\boldsymbol{r}^T\boldsymbol{r})} \\
\quad \textbf{if } norm/norm0 < \varepsilon \textbf{ then} \\
\quad\quad \mathrm{break} \\
\quad \textbf{end if} \\
\quad \rho\mathrm{prev} := \rho \\
\textbf{end for}
\end{array}
$$

Parallelization of CG Method

- Parallelized by **row-wise one-dimensional partitioning** of matrix A



$\boldsymbol{x} := \mathrm{Allgather}(\boldsymbol{x}_l)$
$\boldsymbol{r}_l := \boldsymbol{b}_l - \boldsymbol{A}_l\boldsymbol{x}$
$d_t := \boldsymbol{r}_l^T\boldsymbol{r}_l$
$norm0 := \mathrm{sqrt}(\mathrm{AllreduceSum}(d_t))$
for $k := 1, 2, \cdots$ **do**
  $\rho_t := \boldsymbol{r}_l^T\boldsymbol{r}_l$
  $\rho := \boxed{\mathrm{AllreduceSum}(\rho_t)}$
  if $k = 1$ **then**
    $\boldsymbol{p}_l := \boldsymbol{r}_l$
  else
    $\beta := \rho/\rho\mathrm{prev}$
    $\boldsymbol{p}_l := \beta\boldsymbol{p}_l + \boldsymbol{r}_l$
  end if
  $\boldsymbol{p} := \boxed{\mathrm{Allgather}(\boldsymbol{p}_l)}$
  $\boldsymbol{q}_l := \boldsymbol{A}_l\boldsymbol{p}$
  $\alpha_t := \rho/(\boldsymbol{p}_l^T\boldsymbol{q}_l)$
  $\alpha := \boxed{\mathrm{AllreduceSum}(\alpha_t)}$
  $\boldsymbol{x}_l := \alpha\boldsymbol{p}_l + \boldsymbol{x}_l$
  $\boldsymbol{r}_l := -\alpha\boldsymbol{q}_l + \boldsymbol{r}_l$
  $d_t := \boldsymbol{r}_l^T\boldsymbol{r}_l$
  $norm := \mathrm{sqrt}(\boxed{\mathrm{AllreduceSum}(d_t)})$
  if $norm/norm0 < \varepsilon$ **then**
    break
  end if
  $\rho\mathrm{prev} := \rho$
end for

Parallelization of CG Method

- Parallelized CG method requires **collective communications** among all processes
  1. **Allgather** : Gathering required vector data for SpMV
  2. **Allreduce**: Reduction for having the summation of the local dot product
- Implemented collective communications are utilized.

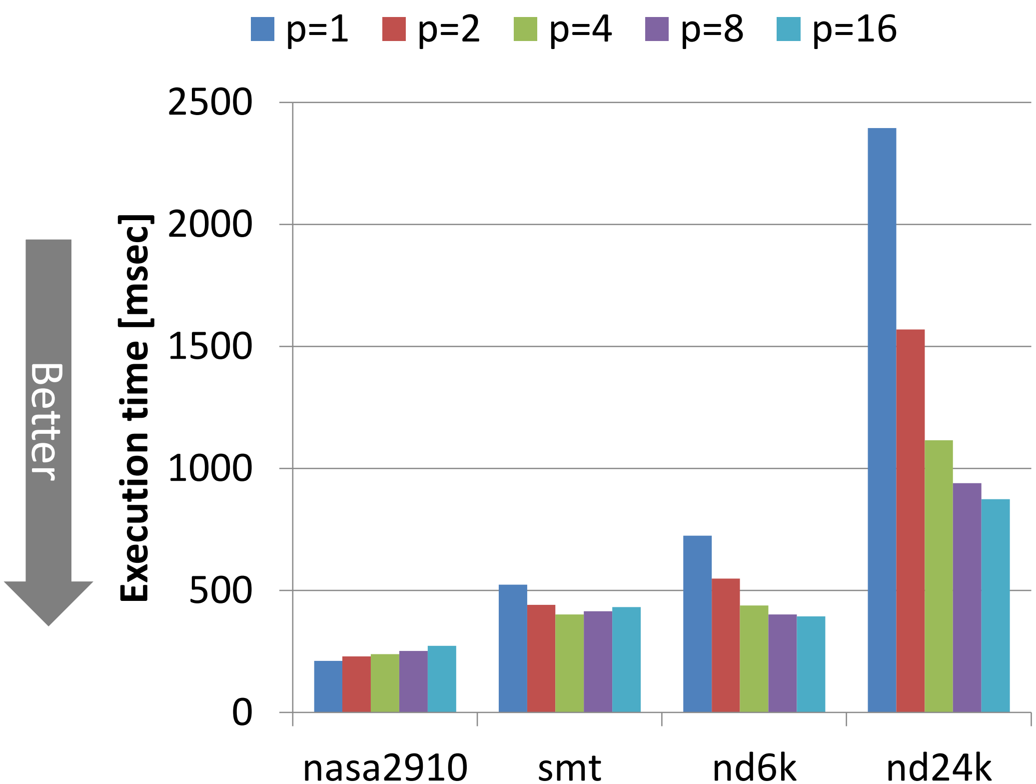
$$
\begin{aligned}
&\boldsymbol{x} := \mathrm{Allgather}(\boldsymbol{x}_l)\\
&\boldsymbol{r}_l := \boldsymbol{b}_l - \boldsymbol{A}_l\boldsymbol{x}\\
&d_t := \boldsymbol{r}_l^T\boldsymbol{r}_l\\
&norm0 := \mathrm{sqrt}(\mathrm{AllreduceSum}(d_t))\\
&\textbf{for } k := 1, 2, \cdots \textbf{ do}\\
&\quad \rho_t := \boldsymbol{r}_l^T\boldsymbol{r}_l\\
&\quad \rho := \boxed{\mathrm{AllreduceSum}(\rho_t)}\\
&\quad \textbf{if } k = 1 \textbf{ then}\\
&\quad\quad \boldsymbol{p}_l := \boldsymbol{r}_l\\
&\quad \textbf{else}\\
&\quad\quad \beta := \rho/\rho\mathrm{prev}\\
&\quad\quad \boldsymbol{p}_l := \beta\boldsymbol{p}_l + \boldsymbol{r}_l\\
&\quad \textbf{end if}\\
&\quad \boldsymbol{p} := \boxed{\mathrm{Allgather}(\boldsymbol{p}_l)}\\
&\quad \boldsymbol{q}_l := \boldsymbol{A}_l\boldsymbol{p}\\
&\quad \alpha_t := \rho/(\boldsymbol{p}_l^T\boldsymbol{q}_l)\\
&\quad \alpha := \boxed{\mathrm{AllreduceSum}(\alpha_t)}\\
&\quad \boldsymbol{x}_l := \alpha\boldsymbol{p}_l + \boldsymbol{x}_l\\
&\quad \boldsymbol{r}_l := -\alpha\boldsymbol{q}_l + \boldsymbol{r}_l\\
&\quad d_t := \boldsymbol{r}_l^T\boldsymbol{r}_l\\
&\quad norm := \mathrm{sqrt}(\boxed{\mathrm{AllreduceSum}(d_t)})\\
&\quad \textbf{if } norm/norm0 < \varepsilon \textbf{ then}\\
&\quad\quad \mathrm{break}\\
&\quad \textbf{end if}\\
&\quad \rho\mathrm{prev} := \rho\\
&\textbf{end for}
\end{aligned}
$$

CG Method Performance: Target Sparse Matrices

- Sparse matrices are from Univ. Florida Sparse Matrix Collection
- Matrix size (#Rows) is 1,000s to 10,000s

Matrix Name	nasa2910	smt	nd6k	nd24k
#Rows (N)	2,910	25,710	18,000	72,000
#Non-zero (nnz)	174,296	3,753,184	6,897,316	28,715,634
nnz/N	59.9	146.0	383.2	398.8

CG Method Performance



Matrix name	nasa2910	smt	nd6k	nd24k
#Rows (N)	2,910	25,710	18,000	72,000

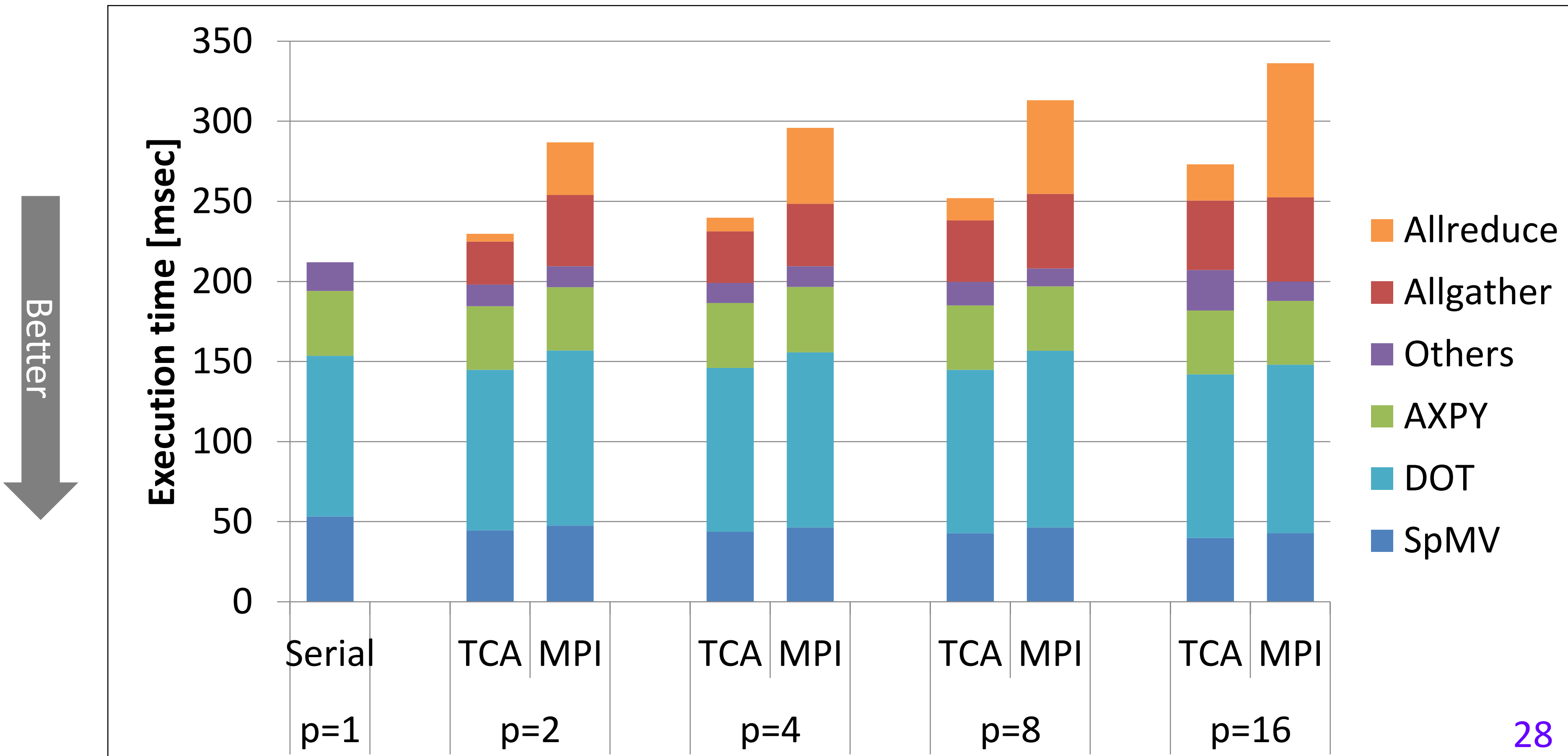
- Time for 1,000 iterations
  - Allgather is implemented with recursive doubling
  - Allreduce is implemented with dissemination algo.
- For **nd6k, nd24k**, parallelization yields **improvement**.
- For **smt**, using 4 processes is the fastest.
- For **nasa2910**, parallelization **deteriorates the performance**.

CG Method Performance: Time breakdown (nasa2910)

N=2,910, nnz=174,296

Breakdown of rank0

- **TCA is faster than MPI**, but performance does not scale

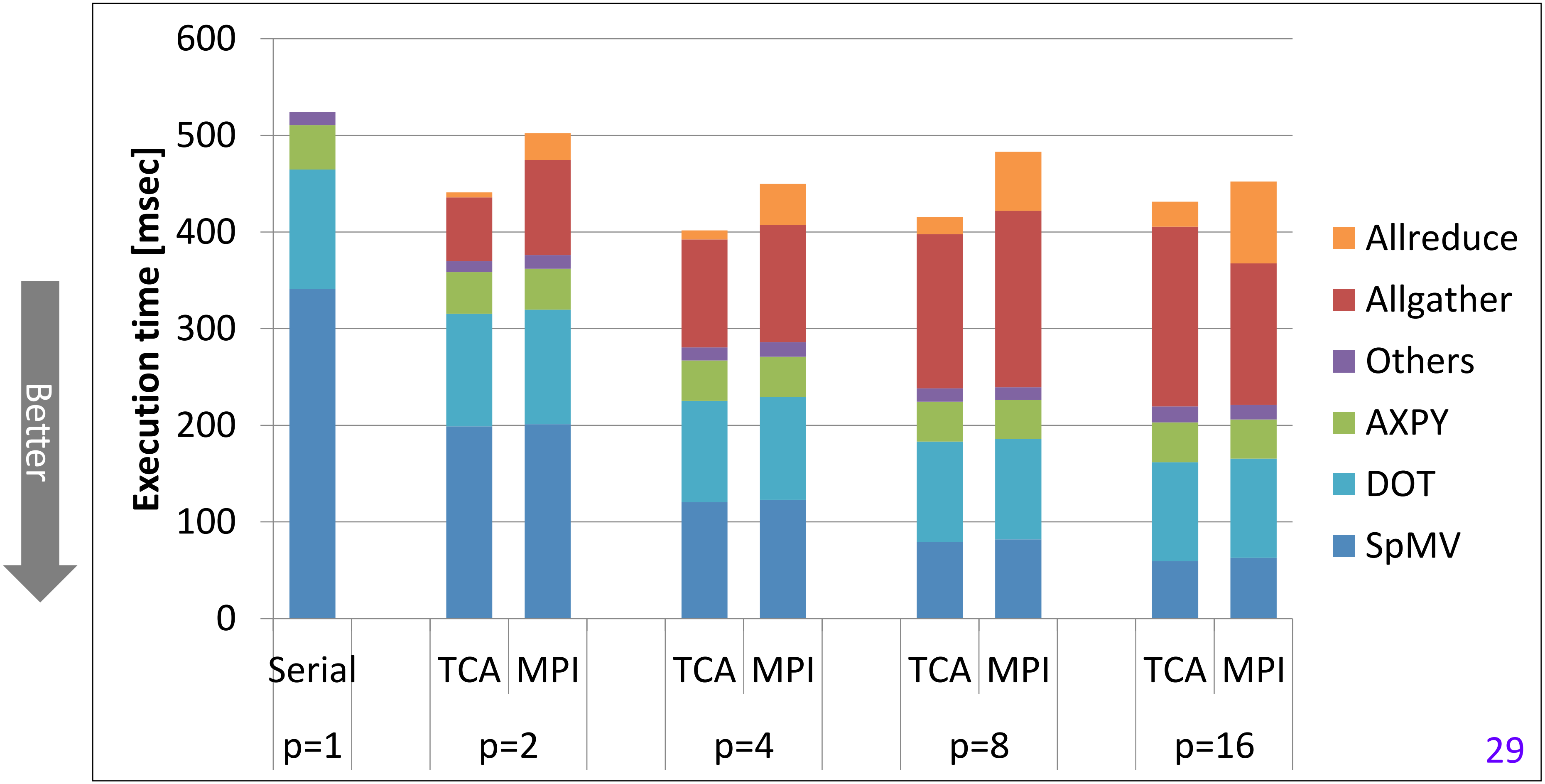


CG Method Performance: Time breakdown (smt)

N=25,710, nnz=3,753,184

Breakdown of rank0

- **TCA improves the performance.**

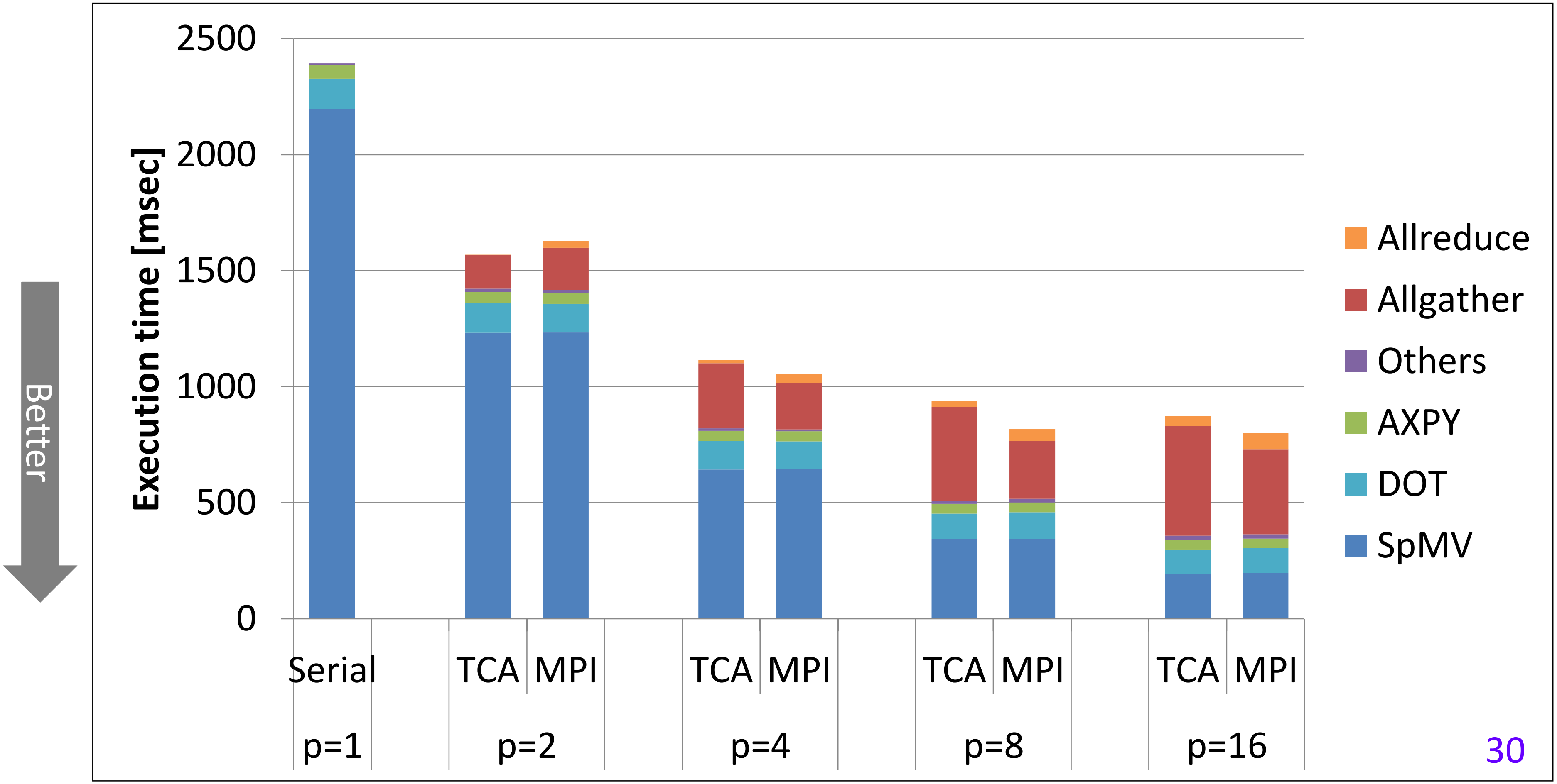


CG Method Performance: Time breakdown (**nd24k**)

N=72,000, nnz=28,715,634

Breakdown of rank0

- Performance scale well, but **TCA is not faster than MPI.**



Discussion

Matrix size	Small (1,000s)	Medium (10,000s)	Large
Performance improvement by TCA	**Large**	**Not-so-bad**	**No**
Strong scalability	**No**	**Not-so-bad**	**High**

- Implementing CG method with one-dimensional partitioning is not very suitable for TCA utilization.
  - We plan to implement and evaluate CG method with two dimensional partitioning.

Conclusion

- Collective communication using TCA/PEACH2's low latency communication improves the performance for small sizes.
- TCA improves the performance of CG method under specific conditions (10,000s rows of matrix).
- We will continue the research on TCA
- Future work:
  Making performance models to predict impact of TCA utilization to the performance.